Structural Investigation of Large Zincferrocenedicarboxylate Clusters

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Introduction: A recent new approach in the preparation of robust framework involves the employment of bis- and tris bidentate organic linkers such as 1,4-benzenedicarboxylate [1]. In this series, dark red crystals of zincferrocenedicarboxylate have been synthesized and characterized by single crystal synchrotron X-ray diffraction. $Zn_3(Fec)_3.(DMF)_2(H_2O)_3$ (where $FecH_2$ is 1.1'-Ferrocenedicarboxylic acid and DMF is Dimethylformamide) is monoclinic, space group $P2_1/n$ with a = 14.990(1), b = 22.606(2), c = 22.994(1) Å, β = 98.010(1)°. The structure consisting of 118 atoms has two types of Zn coordination, four zinc sites have tetrahedral and two have octahedral coordination. Each cluster consists of Zn octahedra sharing a corner with two other Zn tetrahedra. Two such units are capped by six-ferrocene dicarboxyalate in a bidentate fashion. The clusters are held in position by hydrogen bonds with water molecules and DMF.

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References: [1] M. Eddaoudi, H.Li, and O.M. Yaghi. (2000) J. Am. Chem. Soc.,**122**, 1391

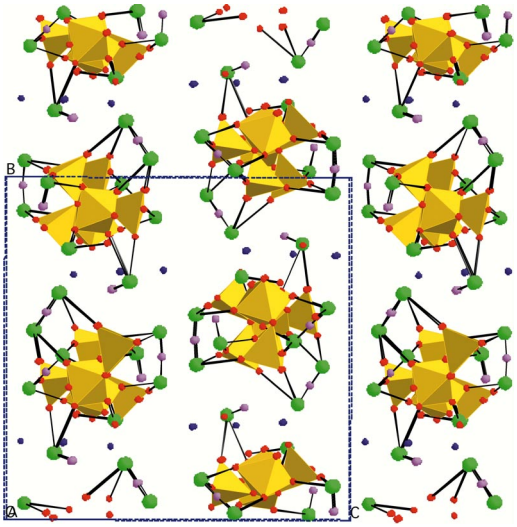

Figure 1. Polyhedral representation of zincferrocenedicarboxylate clusters. 1,1' ferrocenedicarboxylate units (purple and green) cap yellow tetrahedra and octahedra of zinc. The ferrocene units are shown here with 2 carbons attached to an iron for clarity. Blue spheres represent water and DMF, bonded to these clusters by H-bonds. The red spheres represent oxygen atoms.